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TITLE **TODA LATTICE WITH TRANSVERSE DEGREEE OF FREEDOM**

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TODA LATTICE WITH TRANSVERSE DEGREE OF FREEDOM

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ABSTRACT

A transverse degree of freedom is introduced in the Toda lattice. The corresponding continuum approximations are discussed.

INTROUDUCTION

One of the few integrable discrete systems is the nonlinear spring and mass chain introduced by Toda [1]. Its integrability was demonstrated by Flaschka [2] and effective analytical technique based on the spectral transform was developed subsequently [3]. Many theoretical and numerical studies of perturbed Toda lattices have been reported, see [4] e.g.. Recently, the Toda lattice has been applied to model the propagation of longitudinal waves along DNA [5]. Solitons were found to form spontaneously at physiological temperatures. In a more realistic model of DNA also transverse degrees of freedom must be taken into account. Thus a two chain model of DNA was

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treated by statistical mechanics methods in [6] with Morse potentials representing the H-bonds in the base pairs. Here, as a first step, we formulate the Toda lattice model for one strand with a transverse degree of freedom. The continuum approximations of the resulting equations and their solutions are investigated. Computer studies of the lattice dynamics will be presented elsewhere.

FORMULATION OF THE MODEL

We consider a one-dimensional lattice with lattice constant ℓ and N lattice points. At each lattice point we place identical masses (base pairs), m. The longitudinal and transverse displacements from the equilibrium positions are given by $y_1, y_2, \cdots, y_N$ and $v_1, v_2, \cdots, v_N$, respectively. In the case of a circular arrangement of the N masses (corresponding to a circular DNA molecule) we get the periodic boundary conditions for the displacements as function of time, t,

$$y_{n+N}(t) = y_n(t), \;\; v_{n+N}(t) = v_n(t), \;\; n = 1, 2, \cdots, N \quad . \tag{1}$$

The elongation (or compression) of the spring connecting the n'th and (n+1)'th masses is given by

$$r_n = [(\ell + y_{n+1} - y_n)^2 + (v_{n+1} - v_n)^2]^{\frac{1}{2}} - \ell \quad . \tag{2}$$

$r_n = 0$ when the length of the spring is equal to the lattice constant. Note that $r_0 = r_N$ is the elongation of the spring connecting the 1st and the N'th masses. The Toda potential [1] is given by

$$V(r_n) = \frac{a}{b}\,[\exp(-br_n) + 1] + ar_n \quad , \tag{3}$$

where a and b are constants. The Hamiltonian for the Toda chain becomes

$$H = \sum_{n=1}^{N} \frac{1}{2}\, m\,(\dot{y}_n^2 + \dot{v}_n^2) + V(r_n) \quad , \tag{4}$$

where dot denotes differentiation with respect to time. The dynamical equations become

$$m\ddot{y}_n = -V'(r_n)\,\frac{\partial r_n}{\partial y_n} - V'(r_{n-1})\,\frac{\partial r_{n-1}}{\partial y_n} \tag{5a}$$

and

$$m\ddot{v}_n = -V'(r_n)\,\frac{\partial r_n}{\partial v_n} - V'(r_{n-1})\,\frac{\partial r_{n-1}}{\partial v_n} \quad . \tag{5b}$$

There are two characteristic lengths in the model, ℓ and $1/b$, and we shall denote their ratio $\beta = \ell b$. Furthermore, we introduce the mass density $\rho = m/\ell$. A characteristic time is $\ell\sqrt{\rho/a}$. Parameter values for DNA [5] are given in Table 1.

$\ell = 3.4 \quad \times 10^{-10}$	m $\quad \beta = \ell b \quad = 21$
$a = 5.13 \quad \times 10^{-10}$ N	$\rho = m/\ell = 3.77 \times 10^{-15}$ kg/m
$b = 6.18 \quad \times 10^{10} \quad m^{-1}$	$\ell\sqrt{\rho/a} = 9.2 \times 10^{-13}$ s
$m = 1.282 \times 10^{-24}$ kg	

Table 1. Parameter values for DNA [5].

It is convenient to introduce the longitudinal and transverse strains

$$\epsilon^{\alpha}\, u_n = (y_{n+1} - y_n)/\ell \tag{6a}$$

and

$$\epsilon^{\gamma}\, w_n = (v_{n+1} - v_n)/\ell \quad , \tag{6b}$$

where ϵ is an indicator of smalness. We shall consider asymptotic expansions of Eq. (5) for small elongations in four cases:

i) longitudinal strain larger than transverse strain ($\alpha = 1$, $\gamma = 2$)

ii) longitudinal and transverse strain of same order of magnitude ($\alpha = \gamma = 1$)

iii) longitudinal strain smaller than transverse strain ($\alpha = 2$, $\gamma = 1$)

iv) longitudinal strain much smaller than transverse strain ($\alpha = 3$, $\gamma = 1$).

The resulting equations have the form

$$\epsilon^{\alpha} \frac{\ell^2 \rho}{a} \ddot{u}_n = U_{n+1} - 2U_n + U_{n-1} \tag{7a}$$

and

$$\epsilon^{\gamma} \frac{\ell^2 \rho}{a} \ddot{w}_n = W_{n+1} - 2W_n + W_{n-1} \tag{7b}$$

with

$$U_n \simeq (1 - \exp(-\, br_n))\,(1 - \epsilon^{2\gamma} w_n^2/2) \tag{7c}$$

and

$$W_n \simeq \epsilon^{\alpha}(1 - \exp(-br_n))\, w_n \quad . \tag{7d}$$

In the case where not only $r_n/\ell < 1$, but also $r_n\, b = \beta\, r_n/\ell < 1$ we may truncate the Toda potential to

$$V(r_n) \simeq \frac{a}{b}\left[\frac{(br_n)^2}{2} - \frac{(br_n)^3}{6}\right] \tag{8}$$

and arrive at the Boussinesq approximations given in Table 2.

Case	α,γ	U_n	W_n
i	1,2	$\epsilon\beta u_n - \epsilon^2 \frac{\beta^2}{2} u_n^2$	$\epsilon^3 \beta u_n w_n$
ii	1,1	$\epsilon\beta u_n - \epsilon^2 \left[\frac{\beta^2}{2} u_n^2 - \frac{\beta}{2} w_n^2\right]$	$\epsilon^2 \beta u_n w_n$
iii	2,1	$\epsilon^2\beta (u_n + \frac{1}{2} w_n^2)$ $- \epsilon^4\left[\frac{\beta^2}{2} u_n + \beta(1 + \frac{\beta}{2}) u_n w_n^2 + \frac{\beta}{8} (3 + \beta) w_n^4\right]$	$\epsilon^3 \beta(u_n + \frac{1}{2}w_n^2) w_n$
iv	3,1	$\epsilon^2 \frac{\beta}{2} w_n^2 + \epsilon^3 \beta u_n$	$\epsilon^3 \frac{\beta}{2} w_n^3$

Table 2. Asymptotic expansions of U_n and W_n (Eq. (7)) for small longitudinal and transverse excitations.

CONTINUUM APPROXIMATIONS

In order to derive continuum approximations for the lattice equations (7–8) we follow Collins [7] and Rosenau and Hyman [8]. These authors developed ideas by Kruskal and Zabusky [9] and showed that

$$T(f_{n+1}) - 2T(f_n) + T(f_{n-1}) \to \left[1 - \frac{\ell^2}{12}\frac{\partial^2}{\partial x^2}\right]^{-1} \ell^2 \frac{\partial^2}{\partial x^2} T(f) \quad . \tag{9}$$

Here T is a nonlinear function of $f_n(t) \to f(x,t)$ with $x = n\ell$ in the continuum limit $n \to \infty$, $\ell \to 0$. Identifying $T(f_n)$ with U_n and W_n in Eq. (7) obtain the following continnum approximations for the longitudinal and transverse stains, u(x,t) and w(x,t), in the four cases:

i) $$\frac{\varrho}{a} u_{tt} = \beta u_{xx} - \frac{\beta^2}{2} (u^2)_{xx} + \frac{\varrho}{a}\frac{\ell^2}{12} u_{xxtt} \tag{10a}$$

$$\frac{\varrho}{a} w_{tt} = \frac{\varrho}{a}\frac{\ell^2}{12} w_{xxtt} \tag{10b}$$

ii) $$\frac{\varrho}{a} u_{tt} = \beta u_{xx} - \frac{\beta^2}{2} (u^2)_{xx} + \frac{\beta}{2} (w^2)_{xx} + \frac{\varrho}{a}\frac{\ell^2}{12} u_{xxtt} \tag{11a}$$

$$\frac{\varrho}{a} w_{tt} = \beta(uw)_{xx} + \frac{\varrho}{a}\frac{\ell^2}{12} w_{xxtt} \tag{11b}$$

iii) $$\frac{\varrho}{a} u_{tt} = \beta u_{xx} + \frac{\beta}{2} (w^2)_{xx} + \frac{\varrho}{a}\frac{\ell^2}{12} u_{xxtt} \tag{12a}$$

$$\frac{\varrho}{a} w_{tt} = \frac{\varrho}{a}\frac{\ell^2}{12} w_{xxtt} \tag{12b}$$

and

iv) $$\frac{\rho}{a} u_{tt} = \frac{\beta}{2} (w^2)_{xx} + \beta u_{xx} + \frac{\rho}{a} \frac{\ell^2}{12} u_{xxtt} \qquad (13a)$$

$$\frac{\rho}{a} w_{tt} = \frac{\beta}{2} (w^3)_{xx} + \frac{\rho}{a} \frac{\ell^2}{12} w_{xxtt} \quad . \qquad (13b)$$

Here we have kept terms of order ϵ and ϵ^2 in Eqs. (10–12), and terms of order ϵ, ϵ^2, and ϵ^3 in Eq. (13), and then omitted the ϵ's. In all four cases w(x,t) can be replaced by −w(x,t). The longitudinal strain, u(x,t), does not have this symmetry property.

ON THE SOLUTIONS

In case i) the longitudinal field and the transverse fields decouple. u(x,t) satisfies (10a) which is the improved Boussinesq equation [9]. In the solitonic limit (of infinite periodicity interval and finite velocity) the travelling wave solution to this equation becomes

$$u(x,t) = -\frac{3}{\beta} (s^2-1) \operatorname{sech}^2 \frac{\sqrt{3(s^2-1)}}{s\ell} \left[x - s\sqrt{\frac{\beta a}{\rho}}\, t - x_o\right] \quad . \qquad (14)$$

This compressional travels with the supersonic velocity, $s\sqrt{\beta a/\rho}$ ($s > 1$), $\sqrt{\beta a/\rho}$ being the sound velocity (= 1.69×10^3 m/s for DNA).

Eq. (10b) with the periodicity condition

$$w(x,t) = w(x + jL, t) \qquad j = 1, 2, \cdots \quad , \qquad (15)$$

when $L = N \cdot \ell$, has the trivial solution

$$w(x,t) = \cosh \left[\frac{\sqrt{12}}{\ell} \left[x - \frac{L}{2}\right]\right] T(t) \qquad (16)$$

for j = 1. Here T(t) is an arbitrary function of time. Thus the transverse strain is a standing wave.

In case ii) where the longitudinal and transverse strains are of the same order of magnitude we investigate the ansatz

$$w = Au + B \quad \text{or} \quad u = w/A - B/A \qquad (17a,b)$$

where A and B are constants. Eqs. (11a) and (11b) become identical if we choose

$$A = \pm \sqrt{2+\beta} \text{ and } B = \mp \sqrt{2+\beta}/(1+\beta) \quad . \qquad (18a,b)$$

The resulting equation is

$$\frac{\rho}{a} u_{tt} = -\frac{\beta}{1+\beta} u_{xx} + \beta(u^2)_{xx} + \frac{\rho}{a} \frac{\ell^2}{12} u_{xxtt} \qquad (19a)$$

or

$$\frac{\rho}{a} w_{tt} = \frac{\beta}{1+\beta} \pm \frac{\beta}{\sqrt{2+\beta}} (w^2)_{xx} + \frac{\rho}{a}\frac{\ell^2}{12} w_{xxtt} \quad . \tag{19b}$$

For infinite periodicity interval we find the travelling wave solution

$$u(x,t) = \frac{1}{1+\beta}\left[1 + \frac{3}{2}(s^2-1)\,\mathrm{sech}^2 \frac{\sqrt{3(s^2-1)}}{s\ell}\left[x - s\sqrt{\frac{\beta a}{(1+\beta)\rho}}\,t - x_o\right]\right] \tag{20a}$$

or

$$w(x,t) = \pm\frac{3}{2}\frac{\sqrt{2+\beta}}{1+\beta}(s^2-1)\,\mathrm{sech}^2 \frac{\sqrt{3(s^2-1)}}{s\ell}\left[x - s\sqrt{\frac{\beta a}{(1+\beta)\rho}}\,t - x_o\right] \quad . \tag{20b}$$

The longitudinal solitary wave (20a) differs from the uncoupled solitary wave (14) by being elongated instead of compressional, by existing as a superposition to the constant elongation $(1+\beta)^{-1}$ (like a "dark soliton" in the terminology of optical solitons), and by having a velocity, $s\sqrt{\beta a/(1+\beta)\rho}$, which may be smaller than the sound velocity (for $1 < s < 1.024$ in the case of DNA where $\beta = 21$). Thus the ansatz (17) that the longitudinal and transverse strains travel together (with the same velocity) makes this hybrid wave travel slower than the uncoupled longitudinal strain wave by a factor $\sqrt{1+\beta}$ and faster than the uncoupled transverse strain wave which is a standing wave with zero velocity.

In <u>case iii</u>) the transverse strain is again a standing wave (solution to Eq. (12b) which is identical to (10b)). This wave acts as a source term in the linear dispersive wave equation (12a) for the longitudinal strain which can be solved by separation of variables.

In <u>case iv</u>) the wave equation for the longitudinal strain (13a) is identical to Eq. (12a). However, the transverse strain in the source term is given by the nonliner equation (13b) for which we have obtained solutions by separation of variables

$$w(x,t) = X\left[\frac{\sqrt{12}}{\ell}x\right] T\left[\frac{1}{\ell}\sqrt{\frac{6\beta a}{\rho}}\,t\right] \quad , \tag{21}$$

yielding the differential equations

$$X'' - C = -\Lambda(x^3)'' \tag{22a}$$

and

$$T^3 = \Lambda T'' \tag{22b}$$

for the functions X and T. Here prime denotes differentiation with respect to the arguments, $\frac{\sqrt{12}}{\ell}x$

and $\frac{1}{l}\sqrt{\frac{6\beta a}{\rho}}\,t$, and Λ is the separation constant. Phase plane analysis of the integrated systems.

$$\left.\begin{aligned} X' &= \pm\frac{\sqrt{\frac{3\Lambda}{2}X^4 + X^2 + C_1}}{3\Lambda X^2 + 1} \\ X'' &= \frac{X(1 - 6\ (X')^2}{3\Lambda X^2 + 1} \end{aligned}\right\} \tag{23a}$$

and

$$\left.\begin{aligned} T' &= \pm\sqrt{\frac{1}{2\Lambda}}(T^4 - C_2) \\ T'' &= \frac{T^3}{\Lambda} \end{aligned}\right\} \tag{23b}$$

shows blow up for $\Lambda > 0$. (Example: For the integration constants $(C_1, C_2) = \left[\frac{1}{6\Lambda}, 0\right]$ we get the rational solution

$$w(x,t) = \pm\sqrt{\frac{2\rho}{3\beta a}}\ \frac{x-x_o}{t-t_o} \qquad (24)\ )\quad .$$

For $\Lambda < 0$ bounded solutions to Eq. (13b) are found.

CONCLUSION

For the Toda lattice with a transverse degree of freedom the dynamical equations are derived for spring elongations, which are small compared to the lattice constant, in cases of different orders of magnitude of the ratio between the longitudinal field and the transverse field. Continuum approximation leads to partial differential equations of improved Boussinesq type when the spring elongation is small also compared to the Toda length parameter (1/b). When the longitudinal field is small compared to the transverse field the fields decouple into a supersonic longitudinal solitary wave and a standing transverse wave. When the two fields are of the same order of magnitude a hybrid wave which may be subsonic is found. (The longitudinal wave then has the character of a "dark" compressional solitary wave). The stability of the hybrid wave is presently under investigation. When the transverse field is larger than the longitudinal field, we find a standing transverse wave acting as a source for linear dispersive longitudinal waves. The standing transverse wave may be nonlinear and has been found by separation of variables.

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REFERENCES

[1] M. Toda, Phys. Rep. 18 (1975) 1.

[2] H. Flaschka, Phys. Rev. B 9 (1974) 1924; Prog. Theor. Phys. 51 (1974) 703.

[3] H. Flaschka and D.W. McLaughlin, Prog. Theor. Phys. 55 (1976) 438; W.E. Ferguson, H. Flaschka, and D.W. McLaughlin, J. Comput. Phys. 45 (1982) 157.

[4] B.L. Holian, H. Flaschka, and D.W. McLaughlin, Phys. Rev. A 24 (1981) 2595.

[5] V. Muto, A.C. Scott, and P.L. Christiansen, Phys. Lett. A 136 (1989) 33.

[6] M. Peyrard and A.R. Bishop, Phys. Rev. Lett. 62 (1989) 2755.

[7] M.A. Collins, Chem. Phys. Lett. 77 (1981) 342.

[8] P. Rosenau, Phys. Lett. A 118 (1986) 222; J.M. Hyman and P. Rosenau, Phys. Lett. A 124 (1987) 287.

[9] M.P. Soerensen, P.L. Christiansen, and P.S. Lomdahl, J. Acoust. Soc. Am. 76 (1984) 871; M.P. Soerensen, P.L. Christiansen, and O. Skovgaard, J. Acoust. Soc. Am. 81 (1987) 1718.